LISTING OF AND AMENDMENTS TO CLAIMS:

1. – 49. (canceled)

50. (currently amended) A method for calculating digital calibration filters for a Mass Spectrometry (MS) instrument system, comprising the step of:

obtaining, from a given calibration ~~standard~~ ion with its isotopes, at least one actual mass spectral peak shape function,

specifying mass spectral target peak shape functions within respective mass spectral ranges, and

performing a deconvolution operation between the obtained at least one mass spectral peak shape function and the mass spectral target peak shape functions to obtain at least one digital calibration filter from a result of the deconvolution operation.

51. (previously presented) The method of claim 50, wherein the at least one mass spectral peak shape function can be obtained from a section of a mass spectrum that contains a single isotope peak with no significant overlaps from other isotope peaks.

52. (currently amended) The method of claim 50, wherein said obtaining step comprises the steps of:

calculating, for the given calibration ~~standard~~ ion, relative isotope abundances and theoretical mass locations of the isotopes corresponding thereto;

performing convolution operations on both the calculated relative isotope abundances and measured isotope peak clusters using a same continuous function with a narrow peak width; and

performing a deconvolution operation between the measured isotope peak clusters and calculated isotope peak clusters after said convolution operations to obtain the at least one mass spectral peak shape function in the presence of mutually interfering isotopes.

53. (original) The method of claim 50, wherein the at least one calibration filter comprises at least two calibration filters, and said method further comprises the step of further interpolating between the at least two calibration filters to obtain at least one other calibration filter within a desired mass range.

54. (original) The method of claim 53, wherein said interpolating step comprises the steps of:

collecting the at least two calibration filters as vectors in a matrix for decomposition;

decomposing the matrix that includes the at least two calibration filters;

interpolating between decomposed vectors of the matrix to obtain interpolated vectors; and

reconstructing the at least one other calibration filter using the interpolated vectors.

55. (original) The method of claim 54, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

56. (original) The method of claim 50, wherein any of said steps of performing a deconvolution operation employs at least one of a Fourier Transform and a matrix inversion.

57. (original) The method of claim 52, wherein any of said steps of performing a convolution and deconvolution operation employs at least one of a Fourier Transform, a matrix multiplication, and a matrix inversion.

58. (original) The method of claim 50, wherein said obtaining step further comprises the step of interpolating data corresponding to the mass spectral peak shape functions to obtain at least one other mass spectral peak shape function within a desired mass range.

59. (original) The method of claim 58, wherein said interpolating step comprises the steps of:

collecting the mass spectral peak shape functions as vectors in a matrix for decomposition;

decomposing the matrix that includes the mass spectral peak shape functions;

interpolating between decomposed vectors of the matrix to obtain interpolated vectors; and

reconstructing the at least one other mass spectral peak shape function using the interpolated vectors.

60. (original) The method of claim 59, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

61. (previously presented) The method of claim 58, wherein said performing step comprises the step of performing a deconvolution operation between mass spectral target peak shape functions and one of measured mass spectral peak shape functions and the calculated mass spectral peak shape functions to convert the measured mass spectral peak shape functions and the at least one other mass spectral peak shape function to the mass spectral target peak shape functions within the respective mass spectral ranges; and

wherein said calculating step comprises the step of calculating at least one calibration filter from the deconvolution operation.

62. (original) The method of claim 61, wherein the at least one calibration filter comprises at least two calibration filters, and said method further comprises the step of further interpolating between the at least two calibration filters to obtain at least one other calibration filter within a desired mass range.

63. (original) The method of claim 62, wherein said further interpolating step comprises the steps of:

collecting the at least two calibration filters as vectors in a matrix for decomposition;

decomposing the matrix that includes at least two calibration filters;

interpolating between decomposed vectors of the matrix to obtain interpolated vectors; and

reconstructing the at least one other calibration filter using the interpolated vectors.

64. (original) The method of claim 63, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

65. (original) The method of claim 61, wherein said step of performing a deconvolution operation between the mass spectral target peak shape functions and one of the measured mass spectral peak shape functions and the calculated mass spectral peak shape functions employs at least one of a Fourier Transform and a matrix inversion.

66. (previously presented) The method of claim 50, further comprising the step of pre-aligning mass spectral isotope peaks based on a least squares fit between centroid masses of the calculated relative isotope abundances and those of the measured isotope peak clusters, in a pre-calibration step performed subsequent to said calculating step.

67. (original) The method of claim 50, further comprising the steps of: performing pre-calibration instrument-dependant transformations on raw mass spectral data; and performing post-calibration instrument-dependent transformations on a calculated data set corresponding to a test sample

68. (original) The method of claim 67, wherein said steps of performing pre-calibration instrument-dependent transformations and performing post-calibration instrument-dependent transformations involve respectively creating a pre-calibration banded diagonal matrix and a post-calibration banded diagonal matrix, each nonzero column along a banded diagonal of each of the respective matrices for respectively performing an interpolation function corresponding to the pre-calibration instrument-dependent transformations and the post-calibration instrument-dependent transformations, and said method further comprises the step of creating from the at least one calibration filter a calibration banded diagonal matrix for performing both peak shape and mass axis calibration.

69. (original) The method of claim 68, further comprising the step of multiplying the pre-calibration banded diagonal matrix, the calibration banded diagonal matrix and the post-calibration banded diagonal matrix into a total filtering matrix prior to calibrating a test sample.

70. (original) The method of claim 69, wherein the peak shape and the mass axis calibration are performed by matrix multiplication between the total filtering matrix and the raw mass spectral data, and said method further comprises the step of creating another banded diagonal matrix to estimate mass spectral variances of a calibrated signal, the other banded diagonal matrix having each nonzero element along a banded diagonal equal to a square of a corresponding element in the total filtering matrix.

71. (previously presented) The method of claim 70, further comprising the step of applying a weighted regression operation to calibrated mass spectral data to obtain at least one of integrated peak areas, masses and other mass spectral peak data for the mass spectral peaks.

72. (original) The method of claim 71, wherein weights of the weighted regression operation are proportional to an inverse of the mass spectral variances.

73. (original) The method of claim 70, further comprising the step of applying multivariate statistical analysis to calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

74. (original) The method of claim 50, further comprising the steps of:

performing a pre-calibration mass spacing adjustment from a non-uniformly spaced mass acquisition interval to a uniformly spaced mass interval; and

performing a post-calibration mass spacing adjustment from the uniformly spaced mass interval to a reporting interval.

75. (original) The method of claim 74, wherein said steps of performing the pre-calibration mass spacing adjustment and the post-calibration mass spacing adjustment involve respectively creating a pre-calibration banded diagonal matrix and a post-calibration banded diagonal matrix, each nonzero column along a banded diagonal of each of the respective matrices for respectively performing an interpolation function

corresponding to the pre-calibration mass spacing adjustment and the post-calibration mass spacing adjustment, and said method further comprises the step of creating from the at least one calibration filter a calibration banded diagonal matrix for performing both peak shape and mass axis calibration.

76. (original) The method of claim 75, further comprising the step of multiplying the pre-calibration banded diagonal matrix, the calibration banded diagonal matrix and the post-calibration banded diagonal matrix into a total filtering matrix prior to calibrating a test sample.

77. (original) The method of claim 76, wherein the peak shape and the mass axis calibration are performed by matrix multiplication between the total filtering matrix and raw mass spectral data, and said method further comprises the step of creating another banded diagonal matrix to estimate mass spectral variances of a calibrated signal, the other banded diagonal matrix having each nonzero element along a banded diagonal equal to a square of a corresponding element in the total filtering matrix.

78. (previously presented) The method of claim 77, further comprising the step of applying a weighted regression operation to the calibrated mass spectral data to obtain at least one of integrated peak areas, masses and other mass spectral peak data for the mass spectral peaks.

79. (original) The method of claim 78, wherein weights of the weighted regression operation are proportional to an inverse of the mass spectral variances.

80. (original) The method of claim 77, further comprising the step of applying multivariate statistical analysis to the calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

81. (previously presented) The method of claim 50, further comprising the step of adding the calibration standard into a test sample one of prior to and in real-time through at least one of continuous infusion and online mixing so as to acquire both calibration data and test data in one data acquisition.

82. (currently amended) A method of processing mass spectral data, comprising the steps of:

applying a total filtering matrix to ~~the~~ raw mass spectral data to obtain calibrated mass spectral data,

wherein the total filtering matrix is formed by:

obtaining, from a given calibration ~~standard~~ ion with its isotopes, at least one actual mass spectral peak shape function,

specifying mass spectral target peak shape functions within respective mass spectral ranges, and

performing a deconvolution operation between the obtained at least one mass spectral peak shape function and the mass spectral target peak shape functions to obtain at least one digital calibration filter from a result of the deconvolution operation.

83. (original) The method of claim 82, wherein said applying step further comprises the step of interpolating the raw mass spectral data onto a same mass axis as that required by the total filtering matrix.

84. (original) The method of claim 82, wherein said applying step further comprises the step of interpolating the calibrated mass spectral data onto any desired mass axis different from that given by the total filtering matrix.

85. (previously presented) The method of claim 82, further comprising the step of applying a weighted regression operation to the calibrated mass spectral data to obtain at least one of integrated peak areas, masses and other mass spectral peak data for the mass spectral peaks.

86. (original) The method of claim 85, wherein weights of the weighted regression operation are proportional to an inverse of mass spectral variances.

87. (original) The method of claim 82, further comprising the step of applying multivariate statistical analysis to the calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

88. (currently amended) A method for obtaining at least one actual mass spectral peak shape function, comprising the steps of:

calculating, for a given calibration ~~standard~~ ion, relative isotope abundances and theoretical mass locations of isotopes corresponding to the at least one mass spectral peak;

performing convolution operations on both calculated relative isotope abundances and measured isotope peak clusters using a same continuous function with a narrow peak width; and

performing a deconvolution operation between the measured isotope peak clusters and calculated isotope peak clusters after said convolution operations to obtain the at least one actual mass spectral peak shape function in the presence of mutually interfering isotopes.

89. (previously presented) The method of claim 88, wherein the at least one mass spectral peak shape function is obtained from a section of a mass spectrum that contains at least one of many isotopes from a known ion in a calibration standard.

90. (previously presented) The method of claim 88, wherein any of said steps of performing a convolution and deconvolution operation employs at least one of a Fourier Transform, a matrix multiplication, and a matrix inversion.

91. (previously presented) The method of claim 88, further comprising the step of interpolating data corresponding to the mass spectral peak shape functions to obtain at least one other mass spectral peak shape function within a desired mass range.

92. (previously presented) The method of claim 91, wherein said interpolating step comprises the steps of:

collecting the mass spectral peak shape functions as vectors in a matrix for decomposition;

decomposing the matrix that includes the mass spectral peak shape functions;

interpolating between decomposed vectors of the matrix to obtain interpolated vectors; and

reconstructing the at least one other mass spectral peak shape function using the interpolated vectors.

93. (previously presented) The method of claim 92, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

94. (previously presented) The method of claim 88, further comprising:

specifying mass spectral target peak shape function; and

performing a deconvolution operation between the obtained at least one mass spectral peak shape function and the mass spectral target peak shape functions.

95. (previously presented) The method of claim 94, wherein said performing step comprises the step of performing a deconvolution operation between mass spectral target peak shape functions and one of measured mass spectral peak shape functions and calculated mass spectral peak shape functions to convert measured mass spectral peak shape functions and the at least one other mass spectral peak shape function to the mass spectral target peak shape functions.

96. (previously presented) The method of claim 95, wherein said calculating step comprises the step of calculating at least one calibration filter from the deconvolution operation.

97. (previously presented) The method of claim 96, wherein the at least one calibration filter comprises at least two calibration filters, and said method further comprises the step of interpolating between the at least two calibration filters to obtain at least one other calibration filter within a desired mass range.

98. (previously presented) The method of claim 97, wherein said interpolating step comprises the steps of:

collecting the at least two calibration filters as vectors in a matrix for decomposition;

decomposing the matrix that includes at least two calibration filters;

interpolating between decomposed vectors of the matrix to obtain interpolated vectors; and

reconstructing the at least one other calibration filter using the interpolated vectors.

99. (previously presented) The method of claim 98, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

100. (previously presented) The method of claim 95, wherein said step of performing a deconvolution operation between the mass spectral target peak shape functions and one of the measured mass spectral peak shape functions and the calculated mass spectral peak shape functions employs at least one of a Fourier Transform and a matrix inversion.

101. (previously presented) The method of claim 88, further comprising the step of pre-aligning mass spectral isotope peaks based on a least squares fit between centroid masses of the calculated relative isotope abundances and those of measured isotope peak clusters, in a pre-calibration step performed subsequent to said calculating step.

102. (previously presented) The method of claim 96, further comprising the steps of: performing pre-calibration instrument-dependant transformations on raw mass spectral data; and performing post-calibration instrument-dependent transformations on a calculated data set corresponding to a test sample.

103. (previously presented) The method of claim 102, wherein said steps of performing pre-calibration instrument-dependent transformations and performing post-calibration instrument-dependent transformations involve respectively creating a pre-calibration banded diagonal matrix and a post-calibration banded diagonal matrix, each nonzero element along a banded diagonal of each of the respective matrices for respectively performing an interpolation function corresponding to the pre-calibration instrument-dependent transformations and the post-calibration instrument-dependent transformations, and said method further comprises the step of creating from the at least one calibration filter a calibration banded diagonal matrix for performing both peak shape and mass axis calibration.

104. (previously presented) The method of claim 103, further comprising the step of multiplying the pre-calibration banded diagonal matrix, the calibration banded diagonal matrix and the post-calibration banded diagonal matrix into a total filtering matrix prior to calibrating a test sample.

105. (previously presented) The method of claim 104, wherein the peak shape and the mass axis calibration are performed by matrix multiplication between the total filtering matrix and the raw mass spectral data, and said method further comprises the step of creating another banded diagonal matrix to estimate mass spectral variances of a calibrated signal, the other banded diagonal matrix having each nonzero element along a banded diagonal equal to a square of a corresponding element in the total filtering matrix.

106. (previously presented) The method of claim 105, further comprising the step of applying a weighted regression operation to calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

107. (previously presented) The method of claim 106, wherein weights of the weighted regression operation are proportional to an inverse of the mass spectral variances.

108. (previously presented) The method of claim 105, further comprising the step of applying multivariate statistical analysis to calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

109. (previously presented) The method of claim 88, further comprising the steps of:

performing a pre-calibration mass spacing adjustment from a non-uniformly spaced mass acquisition interval to a uniformly spaced mass interval; and

performing a post-calibration mass spacing adjustment from the uniformly spaced mass interval to a reporting interval.

110. (previously presented) The method of claim 109, wherein said steps of performing the pre-calibration mass spacing adjustment and the post-calibration mass spacing adjustment involve respectively creating a pre-calibration banded diagonal matrix and a post-calibration banded diagonal matrix, each nonzero element along a banded diagonal of each of the respective matrices for respectively performing an interpolation function corresponding to the pre-calibration mass spacing adjustment and the post-calibration mass spacing adjustment, and said method further comprises the step of creating from the at least one calibration filter a calibration banded diagonal matrix for performing both peak shape and mass axis calibration.

111. (previously presented) The method of claim 110, further comprising the step of multiplying the pre-calibration banded diagonal matrix, the calibration banded diagonal matrix and the post-calibration banded diagonal matrix into a total filtering matrix prior to calibrating a test sample.

112. (previously presented) The method of claim 111, wherein the peak shape and the mass axis calibration are performed by matrix multiplication between the total filtering matrix and raw mass spectral data, and said method further comprises the step of creating another banded diagonal matrix to estimate mass spectral variances of a

calibrated signal, the other banded diagonal matrix having each nonzero element along a banded diagonal equal to a square of a corresponding element in the total filtering matrix.

113. (previously presented) The method of claim 112, further comprising the step of applying a weighted regression operation to the calibrated mass spectral data to obtain at least one of integrated peak areas, masses and other mass spectral peak data for the mass spectral peaks.

114. (previously presented) The method of claim 113, wherein weights of the weighted regression operation are proportional to an inverse of the mass spectral variances.

115. (previously presented) The method of claim 112, further comprising the step of applying multivariate statistical analysis to the calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

116. (previously presented) The method of claim 88, further comprising the step of adding the calibration standard into a test sample one of prior to and in real-time through at least one of continuous infusion and online mixing so as to acquire both calibration data and test data in a single mass spectral acquisition.

117. (previously presented) For use with a mass spectrometer having associated therewith a computer for performing data analysis functions of data produced by the mass spectrometer, a computer readable medium readable by said computer, said computer readable medium having thereon computer readable program instructions for performing the method of any one of claims 50 to 116.

118. (previously presented) A mass spectrometer having associated therewith a computer for performing data analysis functions of data produced by the mass spectrometer, the computer performing the method of any one of claims 50 to 116.

119. (new) The method of claim 52 or claim 82, wherein the digital filter, when applied to a mass spectrum, performs at least one of noise filtering, signal averaging, mass calibration, and peak shape adjustment.